

Techniques for solving bound state problems

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1 Introduction

The Hamiltonian of a system of two scalar particles with mass m in a local potential is in the relativistic situation given by

$$H = 2\sqrt{m^2 + p^2} + V(r) \quad (1)$$

We are interested in solving the Schrödinger equation for binding and confining potentials, that are associated with particle exchange.

There are several methods for obtaining bound states. Probably the simplest way is to directly solve the differential equation in configuration space. Unfortunately we cannot use this method in the relativistic case, since we have to deal with a term that contains a square root of the differential operator.

Another possible method is to directly discretize the integral equation in momentum space. This comes down to solving an equation of the form

$$E\psi_i = \sum_j K_{ij}\psi_j. \quad (2)$$

A third method makes use of the variational principle for the energy and expands the eigenstates in terms of basis functions ($\psi = \sum_i a_i \phi_i$). It turns out to be advantageous to be able to calculate the kinetic part of the Hamiltonian in momentum space and the potential part in configuration space.

In this report we will calculate the bound states with both methods. The issues we concentrate on are ease of numerical implementation, accuracy and stability. Both methods are less easy to implement and calculations take up more time compared to the method of directly solving the differential equation. To compare the accuracy of the two methods, we first need to know whether our codes are correct. To check our codes we have made use of several potentials for which the bound state energies and wave functions are known explicitly in the nonrelativistic case. In section 2 we will present these potentials. In the next section we will look in more detail at the numerical implementation of the methods. In section 4 we will give some numerical results in the nonrelativistic case and in the next section we will look at some physical interesting cases. Finally we will give some conclusions in the last section.

2 Exact solutions of potentials in the nonrelativistic case

There are several potentials for which the bound state energies and wave functions are known in the nonrelativistic situation. We have used three of these potentials to check our codes. They are the Coulomb potential, the linear potential and the Hulthén potential. Note that two of these potentials have some features in common with the Yukawa potential: the Coulomb and Hulthén potentials behave like $1/r$ at $r \rightarrow 0$; the Hulthén potential falls off like an exponential as $r \rightarrow \infty$, almost the same as the Yukawa potential

$$V(r) = \frac{\rho}{r} e^{-\mu_Y r}. \quad (3)$$

By looking at this potential, Eq. (3), one realizes immediately that putting $\mu_Y = 0$ reduces the Yukawa potential to the Coulomb potential. The energies of the bound states in the nonrelativistic Coulomb case are known exactly and given by

$$E_n = -\frac{m\rho^2}{4n^2} \quad (4)$$

2.1 The linear potential

In the case of the linear potential ($V(r) = \sigma r$) the eigenvalues are exactly known for $l = 0$ in the nonrelativistic case and can be expressed in terms of the zeros of the Airy function [2]. The eigenvalues are given by

$$E_n = \left(\frac{\sigma^2}{m} \right)^{1/3} \lambda_n \quad (5)$$

where σ is the strength of the potential and λ_n is the n -th zero of the Airy function (see table 5).

2.2 The Hulthén potential

The Hulthén potential has the following form

$$V(r) = \rho \frac{e^{-\mu_H r}}{1 - e^{-\mu_H r}}, \quad (6)$$

where ρ is the strength of the potential. The wave functions are known for this potential in the nonrelativistic case ($l = 0$) and are given by

$$r\psi(r) = u_k(r) = e^{-\alpha_k r} (1 - e^{-\mu_H r}) P_k^{(2\alpha_k/\mu_H, 1)} (1 - 2e^{-\mu_H r}), \quad (7)$$

where α_k is defined as

$$\alpha_k = \frac{-m\rho - (k+1)^2 \mu_H^2}{2(k+1)\mu_H}, \quad (8)$$

$P_k^{(2\alpha_k/\mu_H, 1)}$ is a Jacobi polynomial ?? and the bound state energies are given by

$$E_k = -\frac{\alpha_k^2}{m}. \quad (9)$$

3 Implementation

There are different methods to calculate the bound state energies and wave functions of a system. The methods we present here are chosen for different reasons; ease of implementation, accuracy, speed, stability etc. First we will present the different approaches to calculate bound states. Then we will look in more detail at the methods we use and pay attention to the stability and accuracy of these methods.

3.1 Different approaches to calculate bound states

The first method we mention is the method in which the differential equation is solved step by step. It is very easy to implement. The calculations do not take much time, but it is not very accurate. And unfortunately this method gives problems in the relativistic case.

Discretizing the integral equation is a more accurate method. It is less easy to implement and calculations done using this method take up much more time. This method is not very well suited to all potentials, since all calculations are done in the momentum space representation and we may have to deal with singularities in the potential matrix elements.

The third method we present expands the eigenfunctions in terms of basis functions and does not have this problem. The two parts of the Hamiltonian, the kinetic and potential energies respectively, are calculated in either momentum space or configuration space, whatever is more convenient. This method also gives a better accuracy than the first method, but it also takes more time to do the calculations.

3.1.1 Directly solving the differential equation

Probably the simplest way to determine the bound states of a nonrelativistic system is to directly solve the differential equation. We have done this by reducing the Schrödinger equation to a set of coupled first order differential equations and solve them using the Runge-Kutta method [1]. This method is only simple to implement for a nonrelativistic system. For a relativistic system it becomes much more difficult or even impossible to calculate the bound states, since we have to deal with a term that contains a square root of the differential operator.

3.1.2 Discretized integral equation

The radial part of the Schrödinger equation in spherical coordinates is given by

$$\left(-\frac{\hbar^2}{m} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{mr^2} + V(r) \right) \psi_l(r) = E \psi_l(r), \quad (10)$$

where l is the orbital angular momentum quantum number and $\psi_l(r)$ is the radial part of the total wave function which is defined as

$$\Psi(\vec{r}) = \psi_l(r) Y_{lm}(\hat{r}) = \frac{u_l(r)}{r} Y_{lm}(\hat{r}). \quad (11)$$

We can also write Eq. (10) in the momentum space representation. We then find the integral equation

$$\frac{p^2}{m} \tilde{\psi}_l(p) + \int_0^\infty dq q^2 \tilde{V}_l(p, q) \tilde{\psi}_l(q) = E \tilde{\psi}_l(p). \quad (12)$$

Here $\tilde{\psi}_l(p)$ is the Fourier transform of the function $\psi_l(r)$ and $\tilde{V}_l(p, q)$ is the Fourier transformed potential.

Since this integral equation cannot be solved in closed form, we apply a suitable Gaussian integration rule, with abscissas q_j and weights w_j and approximate the integral by a finite sum. We first transform the integration variable q to a variable x , so that the integration interval changes from $[0, \infty)$ to $[-1, 1)$. This is done by the transformation

$$q(x) = C \frac{1+x}{1-x}, \quad (13)$$

where C is a positive scaling parameter. Because of this transformation, the integrand contains an additional factor, the Jacobian $dq(x)/dx$.

Now that we have approximated the integral by this finite sum, we can take the momentum variable p equal to the abscissas. By doing this we obtain an eigenvalue equation in matrix form, which has the following form when we choose a total of N abscissas:

$$\sum_{j=1}^N K_{ij} \tilde{\psi}_l(q_j) = E \tilde{\psi}_l(q_i), \quad (14)$$

where the matrix-elements K_{ij} of the matrix K are given by:

$$K_{ij} = \frac{q_j^2}{m} \delta_{ij} + \tilde{w}_j q_j^2 \tilde{V}_l(q_i, q_j) \quad (15)$$

with $\tilde{w}_j = (dq(x_j)/dx_j)w_j$.

The matrix equation (14) would be easier to solve if the matrix would be symmetric. Left-multiplying the matrix equation with a diagonal matrix D , with elements $D_{ij} = q_j \delta_{ij} / \sqrt{\tilde{w}_j}$, and inserting the identity $D^{-1}D$ between the matrix K and the column vector $\tilde{\psi}_l$ gives us a symmetric matrix $\tilde{K} = DKD^{-1}$. The matrix elements \tilde{K}_{ij} are given by

$$\tilde{K}_{ij} = \frac{q_j^2}{m} \delta_{ij} + \sqrt{\tilde{w}_i \tilde{w}_j} v_l(q_i, q_j) \quad (16)$$

for the nonrelativistic situation, and

$$\tilde{K}_{ij} = 2\sqrt{q_j^2 + m^2} \delta_{ij} + \sqrt{\tilde{w}_i \tilde{w}_j} v_l(q_i, q_j) \quad (17)$$

for the relativistic situation, with $v_l(p, q) = pq \tilde{V}_l(p, q)$. The matrix equation we solve in this approach is given by

$$\sum_{j=1}^N \tilde{K}_{ij} \tilde{u}_l(q_j) = E \tilde{u}_l(q_i), \quad (18)$$

where \tilde{u}_l is the eigenvector, whose j -th element is given by $\sqrt{\tilde{w}_j} q_j \tilde{\psi}_l(q_j)$.

3.1.3 Expanding the eigenfunctions in terms of basis functions

In the third approach the eigenvalues are calculated through expanding the eigenfunctions in terms of basis functions. The basis we use in this approach is the one first introduced by Olsson [3] and Weniger [4]. The basis functions are known in this basis in both configuration and momentum space. In configuration space they are given by

$$\psi_{k,l}(r) = N_{kl} (2\mu r)^l e^{-\mu r} L_k^{(2l+2)}(2\mu r), \quad (19)$$

where the normalization is given by

$$N_{kl} = \sqrt{\frac{k!(2\mu)^3}{(k+2l+2)!}} \quad (20)$$

and $L_k^{(2l+2)}(2\mu r)$ is an associated Laguerre polynomial. In the momentum space representation the basis functions are given by

$$\tilde{\psi}_{k,l}(p) = \tilde{N}_{kl} p^l \left(\frac{\mu}{p^2 + \mu^2} \right)^{l+2} P_k^{(l+3/2, l+1/2)} \left(\frac{p^2 - \mu^2}{p^2 + \mu^2} \right), \quad (21)$$

with $P_k^{(\alpha, \beta)}(x)$ a Jacobi polynomial and the normalization constant is

$$\tilde{N}_{kl} = \frac{2\sqrt{\mu k!(k+2l+2)!}}{\Gamma(k+l+3/2)}. \quad (22)$$

The first five wave functions are plotted in Fig. 1 in both configuration and momentum space. Note that these functions differ from the familiar Coulomb and harmonic oscillator basis functions. Ref. [4] gives the mathematical details including the proof of completeness of the basis.

With these basis functions the matrix element of the potential between the initial and final states is calculated in configuration space. As an example we will calculate the matrix elements for the Yukawa potential. Other potentials are treated in a similar way. The angular part of this matrix element reduces to the product of two Kronecker delta functions. The more interesting part for us is the part that depends on the radial coordinates; which looks like

$$\int_0^\infty dr u_{k_i l_i}^*(r) \frac{\exp(-\mu_Y r)}{r} u_{k_j l_j}(r). \quad (23)$$

The integrand can be rewritten in a somewhat different form. This is done by first making the following substitution for the reduced radial wave function

$$u_{kl}(r) = N_{kl} L_k^{(2l+2)}(2\mu r) r^{l+1} e^{-\mu r} = \bar{u}_{kl}(r) e^{-\mu r}, \quad (24)$$

where $\bar{u}_{kl}(r)$ is a polynomial. Note that the (reduced) radial wave functions behave like r^{l+1} . When we make this substitution, we find for Eq. (23)

$$\int_0^\infty dr \frac{1}{r} \exp(-(2\mu + \mu_Y)r) \bar{u}_{k_i l_i}^*(r) \bar{u}_{k_j l_j}(r). \quad (25)$$

An integral of the form

$$\int_0^\infty dx e^{-x} f(x), \quad (26)$$

where $f(x)$ is a polynomial, can be estimated to the order of machine precision using Gauss-Laguerre integration. The expression in Eq. (25) can be written in the desired form by first making the substitution $x = (2\mu + \mu_Y)r$. Discretizing the equation and then making another substitution $r_j = x_j/(2\mu + \mu_Y)$ gives the desired form:

$$\sum_k \bar{w}_k \frac{1}{r_k} \bar{u}_{k_i l_i}^*(r_k) \bar{u}_{k_j l_j}(r_k), \quad (27)$$

where \bar{w}_k is given by

$$\bar{w}_k = \frac{w_k}{2\mu + \mu_Y}. \quad (28)$$

The abscissas x_k and weights w_k are obtained according to the Gauss-Laguerre rule.

To calculate the bound states of the Hamiltonian given by Eq. (1) (or its nonrelativistic equivalent), we expand the eigenfunctions in terms of the basis functions, $\psi = \sum_i a_i \psi_i$, of the Olsson basis and rewrite the eigenvalue equation as

$$\sum_j H_{ij} a_j = \sum_j \langle \psi_i | H | \psi_j \rangle a_j = E a_i. \quad (29)$$

3.2 Determining the accuracy of our methods

There are several factors that influence the accuracy of our results. First we should make a distinction between the accuracy obtained through making a mathematical approximation and the accuracy obtained because of numerical reasons. The integrals we need when calculating the matrix elements of the Yukawa potential can be calculated exactly. However, all other integrals are estimated with a mathematical approximation.

Of course the accuracy of our results depends on more than only the accuracy with which we can calculate the integrals. We have looked at the factors that have an influence on the accuracy when we use our second method (discretizing the integral equation). Here we have a ‘scaling’ parameter C , which has an influence on the accuracy. Another factor that influences the accuracy is the number of abscissas we take in our calculation.

In table 1 we give the calculated bound states for one case: $m = 1.0$, $\rho = -2.0$, $\mu_Y = 0.02$ and a scaling parameter $C = 1.1$. We have calculated the bound states for five different numbers of abscissas. From table 1 we see that the bound states converge.

Table 1: Bound state energies for the Yukawa potential with $m = 1.0$, $\rho = -2.0$ and $\mu_Y = 0.02$ calculated with different numbers of abscissas.

k	20 absc.	50 absc.	80 absc.	125 absc.	155 absc.
0	-1.189770	-0.998801	-0.973828	-0.964817	-0.962900
1	-0.279598	-0.221291	-0.215165	-0.213154	-0.212748
2	-0.111285	-0.079688	-0.077067	-0.076322	-0.076185
3	-0.053701	-0.032550	-0.031212	-0.030875	-0.030818
4	-0.028074	-0.012991	-0.012274	-0.012113	-0.012086
5	-0.020798	-0.004369	-0.004007	-0.003934	-0.003923

To see what kind of influence the scaling parameter C has on the bound states, we have calculated the bound states at different C for the case $m = 1.0$, $\rho = -2.0$ and $\mu_Y = 0.02$ and with 155 abscissas. When we look at the results we see that there is a small domain of scaling parameters where the bound states are stable. For scaling parameters that lie outside this stable domain, the calculated bound state energies are larger. In all our calculations using our second method (discretizing the integral equation) we have taken a scaling parameter of $C = 1.1$, which lies in the middle of the stable domain we found.

In a similar way we have looked at the factors that have an influence on the accuracy when we use our third method (expanding the eigenfunctions in terms of basis functions). For this method the number of basis functions we have taken into account has an influence

on the accuracy. The parameter μ is completely free and can be used to tune the basis to the Hamiltonian at hand. Although this ‘scaling’ parameter can thus be considered as a variational one, in practice one should be careful if the integrals one needs to calculate are obtained numerically. Then it turns out that only in a limited range of values μ is of genuinely variational character.

There are several potentials that we have used and for all these potentials we have looked what kind of influence the variables mentioned above have on the results. In this report we will only show it for the Yukawa potential.

We have looked at the influence of the number of basis functions we take into account. This was done for the following choice of parameters, which are given below:

$$m = 1.0, \rho = -2.0, \mu_Y = 0.02, \mu = 0.35$$

We have made an expansion of the eigenfunctions in terms of the first 5, 10, 15 or 20 basis functions; these eigenvalues are given in table 2. We have also calculated the wave functions in both configuration and momentum space, these are given in resp. Figs. 2 and 3.

Table 2: Bound state energies for the Yukawa potential with $m = 1.0$, $\rho = -2.0$ and $\mu_Y = 0.02$ calculated with different numbers of basis functions.

k	5 basis func.	10 basis func.	15 basis func.	20 basis func.
0	-0.9419469833	-0.9605381489	-0.9605921507	-0.9605921507
1	-0.2122372389	-0.2122966051	-0.2122966051	-0.2122966051
2	-0.07603943348	-0.07604002953	-0.07604002953	-0.07604002953
3	-0.02350080013	-0.03075730801	-0.03075850010	-0.03075850010
4	–	-0.01097238064	-0.01205313206	-0.01206004620
5	–	–	-0.002824902534	-0.003842115402

Looking at the values of the bound state energies given in table 2, we see that these converge. Figs. 2 and 3 show that the wave functions are smoother when we take more basis functions into account. From this evidence we conclude that our results can not be taken to be reliable when only a small number of basis functions is used in making the expansion. When comparing the results of the expansion to the other methods we used 20 basis functions.

The ‘scaling parameter’ μ appears in the basis, but it is not a real variational parameter since we cannot calculate the matrix elements of the kinetic energy without making mathematical approximations. For several values of μ_Y in the range between 0 and 1 we have looked at the behaviour of μ . When we look at the values of the ground state energy at one value of μ_Y and different μ , we find the same value (for at least the first six decimal places) of this ground state for $\mu > 0.30$. For $\mu < 0.30$, we find that the ground state is shifted upwards and has the ‘wrong’ value. We also have determined a stable domain in μ where the first five eigenvalues are the same up to at least six decimal places. For all values of μ_Y the stable domain starts at $\mu = 0.30$ and ends at some value say μ_{\max} . These maximum values are given in table 3 for several values of μ_Y .

Table 3: Maximum value of μ for a stable domain at different values of μ_Y .

μ_Y	0.0	0.001	0.002	0.005	0.01	0.02	0.05	0.1	0.2	0.5	1.0
μ_{\max}	0.414	0.545	0.520	0.542	0.476	0.367	0.467	0.663	1.0	1.0	1.0

In most calculations we have done, we have taken a value of $\mu = 0.35$ for the ‘scaling parameter’, which lies in the stable domain we have determined above.

All together we see that both methods (discretizing the integral equation and making an expansion in basis functions) are not as easy to implement as the method of directly solving the differential equation, although it is not extremely difficult either. Both methods have a stable domain in which we find accurate solutions. These domains are different for different potentials. The accuracy of both methods is better than the accuracy reached with directly solving the differential equation. Comparing the two methods, we see that the results found by making an expansion in basis functions are more accurate.

4 Check of the numerical results in the nonrelativistic case

We have first calculated the bound state energies and wave functions in the nonrelativistic situation for some potentials for which we know the solutions. After this we have calculated the bound states of the Yukawa potential in the nonrelativistic case.

4.1 The Coulomb potential

We have calculated the eigenvalues for the Coulomb potential only with the third method. The reason is that the long-range character of the Coulomb potential leads to a singularity in momentum space that is difficult to handle numerically and in configuration space to an uncertainty whether the asymptotic region is reached in the differential equation.

We limited ourselves to making an expansion of the eigenfunctions in 20 basis states and checked that the first five eigenvalues are accurate. In the calculation we have taken the mass $m = 1.0$, the strength of the potential $\rho = -2.0$ and the ‘scaling parameter’ $\mu = 0.35$.

The calculated eigenvalues and the exact eigenvalues of the Coulomb potential are given in table 4 for the first eight eigenvalues.

Table 4: The calculated eigenvalues ($l = 0$) of the Yukawa potential with $\mu_Y = 0$ and the exact eigenvalues of the Coulomb potential.

n	exact	calculated
1	-1.0000000000	-1.0000000000
2	-0.2500000000	-0.2500000000
3	-0.1111111111	-0.1111111641
4	-0.0625000000	-0.0625000000
5	-0.0400000000	-0.0399999619
6	-0.0277777777	-0.0277774334
7	-0.0204081630	-0.0202956199
8	-0.0156250000	-0.0137485265

4.2 The linear potential

We have calculated the bound states for the linear potential only with the method of expanding the eigenfunctions in terms of the Olsson basis functions. The bound states are

calculated in the nonrelativistic situation for $m = 1.0$, $\sigma = 1.0$, $\mu = 0.90900$ and are given in table 5.

Since $\sigma = 1.0$ and $m = 1.0$ the bound states should be equal to the zeros of the Airy function. Comparing the results in table 5 with the zeros of the Airy function, we see that the first excited state is accurate to the seventh decimal. Higher excited states are less accurate; the accuracy decreases to an accuracy of $\approx 1 : 8000$ for the fourth excited state.

Table 5: Zeros of the Airy function and eigenvalues for the nonrelativistic Schrödinger equation with $m = 1$, $\sigma = 1$. The parameter μ in the basis has the value $\mu = 0.909$.

n	Airy zero	eigenvalue
1	2.33810741	2.33810741
2	4.08794944	4.08794976
3	5.52055983	5.52057237
4	6.78670809	6.78687212
5	7.94413359	7.94534443

In this case we have also calculated the wave functions. These are plotted in Fig. 4.

4.3 The Hulthén potential

For the Hulthén potential we have calculated the bound state energies with our third method. In table 6 the calculated and exact bound states are given for the case $m = 1.0$, $\rho = -0.5$ and $\mu_H = 0.1$. As ‘scaling’ parameter we have used here $\mu = 1.0$ and we have made an expansion in terms of the first 20 basis states.

Table 6: Calculated and exact bound state energies for the Hulthén potential for $m = 1.0$, $\rho = -0.5$ and $\mu_H = 0.1$.

k	calculated	exact
0	-6.002500057	-6.002500000
1	-1.322499990	-1.322500000
2	-0.466944456	-0.466944444
3	-0.180624962	-0.180625000
4	-0.062495589	-0.062500000
5	-0.010959864	-0.013611111

We see that the first five calculated and exact bound states agree to at least four decimal places. Only the very weakly bound fifth excited state cannot be determined accurately.

In Fig. 5 the exact wave functions and the wave functions calculated by making an expansion into 20 basis states are plotted in configuration space. We see that the wave functions we have calculated are the same as the exact wave functions. In Fig. 6 the calculated wave functions are plotted in momentum space.

We have also calculated the wave functions by directly solving the differential equation (Fig. 7). Here we have used the bound state energies calculated with the third approach as an input.

Note that the wave functions in Fig. 7 are not normalized. To see whether these wave functions are the same as the exact and calculated ones in Fig. 5 we can look at the location

of the nodes and of the extrema. In table 7 the nodes and extrema are given for the exact wave functions and the wave functions calculated by directly solving the differential equation. Looking at table 7 we see that the nodes and the maxima coincide.

Table 7: Nodes and extrema of the exact wave functions and the calculated wave functions by directly solving the differential equation for the Hulthén potential.

k	nodes		extrema	
	exact	calculated	exact	calculated
0	–	–	0.400	0.400
1	0.8004	0.800 - 0.804	0.304	0.304
			2.098	2.098
2	0.7616 2.8514	0.760 - 0.764 2.848 - 2.852	0.296	0.296
			1.680	1.680
			5.278	5.278
3	0.7501 2.6632 6.3132	0.750 - 0.752 2.660 - 2.664 6.312 - 6.316	0.292	0.292
			1.608	1.608
			4.314	4.312 - 4.316
			10.146	10.140 - 10.148

4.4 The Yukawa potential

In the case of the Yukawa potential (with $\mu_Y \neq 0$ in Eq. (3)) there are no exact solutions known. We do know, however, that the eigenvalues in this case are greater than the corresponding eigenvalues in the Coulomb case. We also know that the eigenvalues should vary smoothly when μ_Y is varied.

To find the stable domain in which we want to calculate the eigenstates, we have varied μ for different values of μ_Y . In all calculations we have used a value of $\mu = 0.35$, which is in the stable domain for all values of μ_Y . Now that we know where the stable domain lies, we have calculated the eigenstates for the Yukawa potential for several values of μ_Y . In every case we have used 20 basis states in the expansion and expect the first five states to be accurate. All the eigenvalues are calculated for a mass $m = 1.0$ and a strength of the potential $\rho = -2.0$. The results are given in table 8.

We see that for small μ_Y there are several bound states. As μ_Y increases, the number of bound states decreases. For $\rho = -2.0$ and $\mu_Y > 1.8$ there are no bound states found at all. The calculated spectra are also plotted in Fig. 8. In these plots we see very clearly that all energies shift upwards, when μ_Y increases.

We have not only looked at the eigenvalues, but also at the wave functions. For one case we give here the eigenvalues and wave functions as we have calculated them with the different methods. The calculated eigenvalues for the case

$$m = 1.0, \rho = -1.0, \mu_Y = 0.02 \quad (30)$$

are given in table 9. Note that only the bound states calculated with the second and third method are given in this table. For the first method (directly solving the differential equation)

Table 8: Eigenvalues ($l = 0$) of the Yukawa potential for different values of μ_Y in the nonrelativistic case $m = 1.0$ and $\rho = -2.0$. (a ‘--’ means a bound state has not been found)

k	$\mu_Y = 0.01$	$\mu_Y = 0.02$	$\mu_Y = 0.05$	$\mu_Y = 0.1$
0	-0.9801490307	-0.9605921507	-0.9036328793	-0.8141160011
1	-0.2305865288	-0.2122966051	-0.1635423899	-0.0998564959
2	-0.0923976898	-0.0760400295	-0.0387051106	-0.0064160824
3	-0.0447121859	-0.0307585001	-0.0061832666	--
4	-0.0233221054	-0.0120600462	--	--

k	$\mu_Y = 0.2$	$\mu_Y = 0.5$	$\mu_Y = 1.0$
0	-0.6536170244	-0.2962340117	-0.0205712318
1	-0.0242156982	--	--

we have used the bound state energies calculated with our third method as an input to calculate the wave functions.

Table 9: Eigenvalues (nonrelativistic) for the case $m = 1.0$, $\rho = -1.0$ and $\mu_Y = 0.02$ calculated by discretizing the integral equation (second method) and making an expansion of the eigenfunctions (third method).

k	integral eqn.	exp. in basis
0	-0.230696	-0.2305848598
1	-0.044726	-0.0447072983
2	-0.012351	-0.0123461485
3	-0.002981	-0.0029529333

Using all three methods, we have calculated the wave functions. In Fig. 9 the wave functions in both configuration space and momentum space are given as they are calculated by expanding the eigenfunctions in terms of the basis functions.

We have also calculated the wave function in momentum space by the method of discretizing the integral equation (Fig. 10).

Finally we have calculated the wave functions in coordinate space by directly solving the differential equation. We have taken the eigenvalues calculated with our third method as input. The wave functions calculated by this method are plotted in Fig. 11.

Looking at this figure, we see that the wave functions at the end show some strange behaviour, that is they do not converge. The reason that these wave functions do not converge is due to the accumulation of errors. Note that the wave functions shown in Fig. 11 are not normalized. When the wave functions calculated with both methods are the same their nodes and extrema must coincide. In table 10 estimates for the nodes and extrema are given.

We see that the zero points of the wave functions lie in the same place, which means that we are dealing with the same wave functions.

Table 10: Nodes and extrema of the first four wave functions of the nonrelativistic Yukawa Hamiltonian calculated with the first method (directly solving the differential equation) and the third method (expanding the eigenfunctions in terms of basis functions). The parameters are $m = 1.0$, $\rho = -1.0$ and $\mu_Y = 0.02$.

k	nodes		extrema	
	solving diff. eqn.	exp. in basis	solving diff. eqn.	exp. in basis
0	–	–	1.98 - 2.01	2.00 - 2.01
1	3.97 - 4.04	4.01 - 4.02	1.50 - 1.53 10.51 - 10.61	1.53 - 1.54 10.56 - 10.58
2	3.82 - 3.88 14.45 - 14.59	3.82 - 3.83 14.50 - 14.51	1.48 - 1.50 8.44 - 8.52 27.28 - 27.50	1.48 - 1.49 8.49 - 8.50 27.28 - 27.33
3	3.73 - 3.79 13.54 - 13.66 33.45 - 33.72	3.78 - 3.79 13.64 - 13.65 33.46 - 33.47	1.47 - 1.50 8.16 - 8.24 22.46 - 22.62	1.46 - 1.47 8.20 - 8.21 22.41 - 22.45

5 Physical interesting cases

The physically more interesting situation is the relativistic situation. For the Yukawa potential we have calculated the bound state energies and wave functions in the relativistic situation. In this case we see that the wave functions collapse above a certain strength of the potential. This collapse occurs only for certain types of potentials.

5.1 The relativistic case

We have done some calculations in the relativistic case for the Yukawa potential. In this situation the bound states are calculated with the method of expanding the eigenfunctions in terms of basis functions only. We have looked at the same case as in the nonrelativistic situation: $m = 1.0$, $\rho = -1.0$ and $\mu_Y = 0.02$. The results are given in table 11. For comparison we have given the nonrelativistic bound states in the same table. The wave functions are plotted in Fig. 12.

Table 11: Calculated bound state energies (relativistic and nonrelativistic) for the Yukawa potential in the case $m = 1.0$, $\rho = -1.0$ and $\mu_Y = 0.02$.

k	relativistic	nonrelativistic
0	-0.3107976913	-0.2305848598
1	-0.0583696365	-0.0447072983
2	-0.0161626339	-0.0123461485
3	-0.0042042733	-0.0029529333

5.2 The collapse of wave functions

It is interesting to look at what happens in the relativistic situation to the bound states and the wave functions when the strength (ρ) of the potential increases. We know that for the Coulomb potential there exists a critical value of the strength above which the wave functions collapse [5, 6]. We expect to find this collapse for the Yukawa potential as well, since this potential is also not bounded from below.

With a variational calculation we are able to estimate this critical value for the Yukawa potential. As the variational wave function we have taken the lowest Olsson wave function (which is the same as the lowest Coulomb wave function). These are given in coordinate space by

$$\psi(r) = \sqrt{4\mu^3} e^{-\mu r} \quad (31)$$

and in momentum space by

$$\tilde{\psi}(p) = \sqrt{\frac{32\mu^5}{\pi}} \frac{1}{(p^2 + \mu^2)^2}. \quad (32)$$

Using these trial functions we can calculate the potential energy exactly:

$$\begin{aligned} V(\mu) &= \int_0^\infty dr r^2 \sqrt{4\mu^3} e^{-\mu r} \rho \frac{e^{-\mu_Y r}}{r} \sqrt{4\mu^3} e^{-\mu r} \\ &= \frac{4\mu^3 \rho}{(2\mu + \mu_Y)^2}. \end{aligned} \quad (33)$$

The kinetic energy is given by the integral

$$\begin{aligned} T(\mu) &= \int_0^\infty dp p^2 \sqrt{\frac{32\mu^5}{\pi}} \frac{1}{(p^2 + \mu^2)^2} 2\sqrt{p^2 + m^2} \sqrt{\frac{32\mu^5}{\pi}} \frac{1}{(p^2 + \mu^2)^2} \\ &= \frac{64\mu^5}{\pi} \int_0^\infty dp \frac{p^2 \sqrt{p^2 + m^2}}{(p^2 + \mu^2)^4}. \end{aligned} \quad (34)$$

In the limit $\mu \rightarrow \infty$ we can estimate the kinetic energy. Defining $\beta = m/\mu$ and $p = \mu x$ and substituting this in Eq. (34), we get

$$\begin{aligned} T(\mu) &= \frac{64\mu}{\pi} \int_0^\infty dx \frac{x^2 \sqrt{x^2 + \beta^2}}{(x^2 + 1)^4} \\ &\sim \frac{64\mu}{\pi} \int_0^\infty dx \frac{x^3}{(x^2 + 1)^4} \\ &= \frac{64\mu}{12\pi}. \end{aligned} \quad (35)$$

In the second step we have taken the limit $\mu \rightarrow \infty$, or $\beta \rightarrow 0$. In this limit, the potential energy becomes:

$$V(\mu) = \frac{4\mu^3 \rho}{4\mu^2} = \rho\mu. \quad (36)$$

For the total Hamiltonian in this limit we find

$$H(\mu) = \frac{16\mu}{3\pi} + \rho\mu. \quad (37)$$

From this Hamiltonian we can determine the critical value, for which the potential is not bounded from below any more.

$$\rho_{crit} = -\frac{16}{3\pi} \approx -1.697652726 \quad (38)$$

A more accurate estimation is given by [5]: $\rho_{crit} = -4/\pi = -1.2732395$.

To see whether this collapse really occurs, we have looked at what happens when we increase the strength ρ and keep all other parameters the same. In Fig. 13 we have plotted the wave functions of the ground state in configuration space for $m = 1.0$, $\mu_Y = 0.02$ and several values of ρ . In Fig. 14 the same is done for the wave functions in the momentum space representation. In both figures we see that the wave functions show some irregularities at larger ρ . For $\rho \lesssim \rho_{crit}$ the wave function is not a smooth function anymore and ceases to be approximated well by our basis. So we get some irregularities due to numerical errors.

To illustrate that the ground state energy drops very fast, we have plotted it in Fig. 15 for different values of ρ and several values of μ_Y . We see that the curves for different μ_Y do not coincide, but relative differences are getting smaller for larger ρ .

This collapse is typical for potentials that are not bounded from below, like the Coulomb and Yukawa potential. To show the difference, we have done the same calculations for the Saxon-Woods potential

$$V(r) = \frac{\rho}{1 + e^{(r-R)/a}}. \quad (39)$$

This potential is bounded from below, which means that the bound state energies cannot drop to infinity. We have calculated the bound state energies and wave functions in both configuration and momentum space for the case

$$m = 1.0, R = 10.0, a = 1.0, \mu = 0.35 \quad (40)$$

and several values of ρ . The bound state energies are given in table 12, in Fig. 16 the wave functions in configuration space are plotted and in Fig. 17 they are plotted in the momentum space representation. Looking at Figs. 16 and 17 we see that the wave functions do not show any irregularities.

Table 12: Bound state energies for the Saxon Woods potential in the relativistic case for $m = 1.0$, $R = 10.0$, $a = 1.0$.

n	$\rho = -0.1$	$\rho = -0.397975$	$\rho = -1.0$	$\rho = -2.0$
0	-0.04328906536	-0.3107855320	-0.8903754950	-1.870764375
1	—	-0.1143078804	-0.6332213879	-1.569842815
2	—	—	-0.3176877499	-1.184906960
3	—	—	-0.03023195267	-0.7476220131

Finally we have plotted the ground state energy versus the strength ρ for the Saxon Woods potential in the same figure with the Yukawa potential (Fig. 15). Comparing these two potentials, we notice that the curve of the Saxon Woods potential goes down smoothly instead of dropping down, as for the Yukawa potential. The reason for this behaviour is that the Saxon Woods potential is bounded from below and does not have a collapse.

6 Conclusion

The easiest way to obtain the bound states is to directly solve the differential equation. This method is very easy to implement and calculations do not take up much time. Unfortunately it is only usefull in the nonrelativistic situation. Beside, it is not very accurate.

In the relativistic situation we use two other methods; discretizing the integral equation and making an expansion in terms of basis functions. For both methods the implementation is more complicated than in the case of directly solving the differential equation, but it is not extremely difficult. Calculations do take up some more time, but this is negligible. And both methods are more accurate than the method of directly solving the differential equation.

A difference between the methods is that the calculations with the method of discretizing the integral equation are done in momentum space only. When making an expansion in terms of basis functions the kinetic and potential energies are seperately calculated in either momentum or configuration space. A consequence of this difference is that the method of discretizing the integral equation is not very wellsuited to all potentials, since we may have to deal with singularities in the potential matrix elements.

After checking our codes with the exact solutions of several potentials, we have calculated the bound state energies and wave functions for the Yukawa potential in the relativistic case. We found a more deeply bound state in the relativistic situation compared to the nonrelativistic one. We have also looked at what happens to the wave functions when the strength of the potential increases. It turned out that there exists a critical value for the strength above which the wave functions collapse. This collapse only occurs for potentials that are not bounded from below; e.g. the Coulomb or Yukawa potential. Potentials that are bounded from below do not show this collapse, since their ground state energies do not drop down to minus infinity. As an example of this kind of potential we have looked at the Saxon Woods potential.

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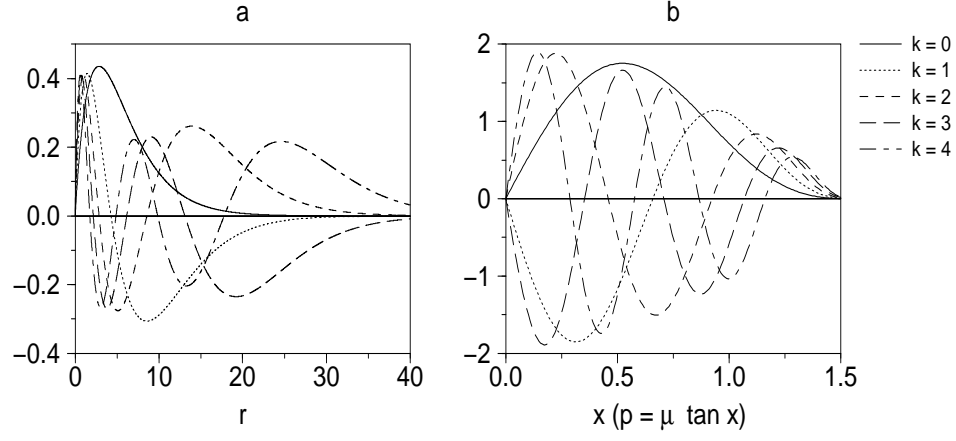


Figure 1: First five basis function in configuration space (a) and momentum space (b).

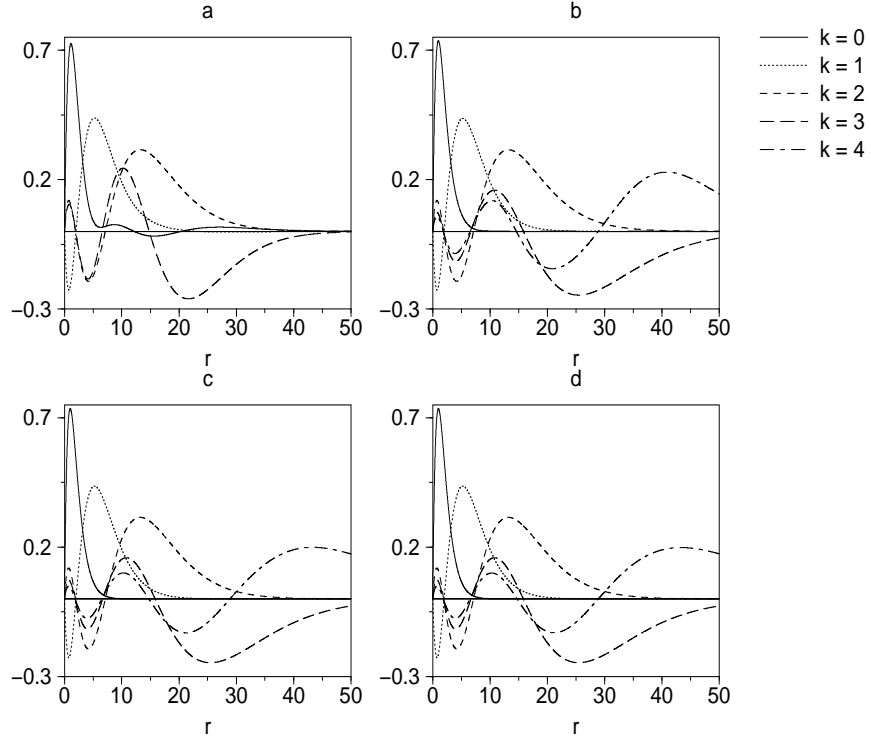


Figure 2: Wave functions in configuration space calculated with (a) 5, (b) 10, (c) 15 or (d) 20 basis functions for the Yukawa potential in the case $m = 1.0$, $\rho = -2.0$ and $\mu_Y = 0.02$.

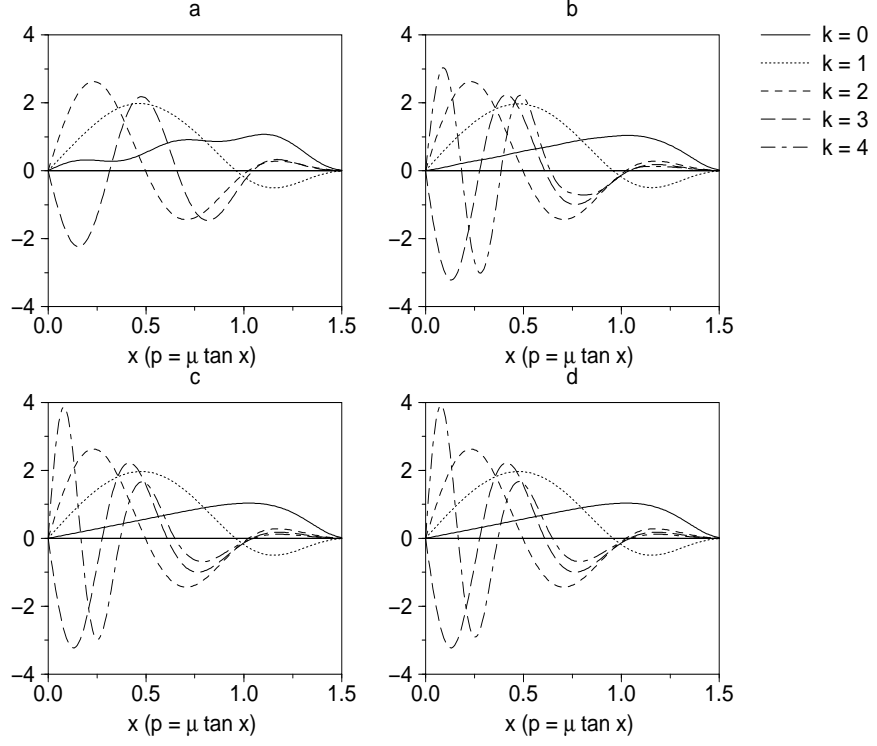


Figure 3: Wave functions in momentum space calculated with (a) 5, (b) 10, (c) 15 or (d) 20 basis functions for the Yukawa potential in the case $m = 1.0$, $\rho = -2.0$ and $\mu_Y = 0.02$.

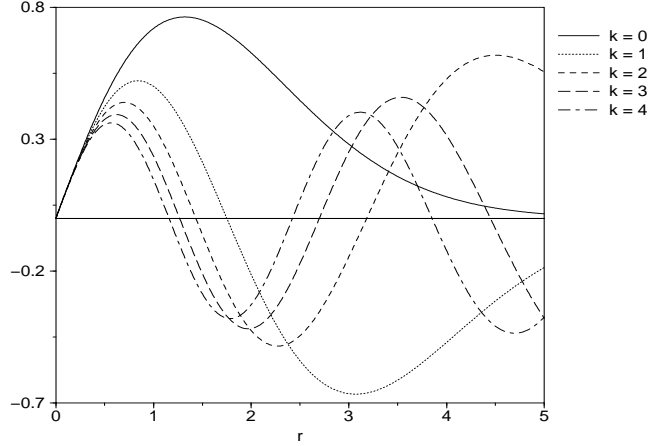


Figure 4: Configuration space wave functions obtained by making an expansion in basis functions. Linear potential with $m = 1.0$, $\sigma = 1.0$.

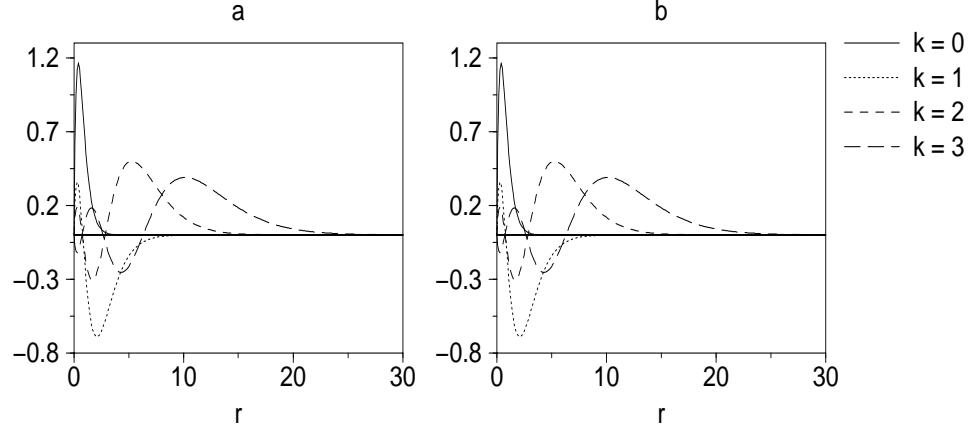


Figure 5: Calculated wave functions (by making an expansion in basis functions) (a) and exact wave functions (b) in configuration space for the Hulthén potential in the case: $m = 1.0$, $\rho = -0.5$ and $\mu_H = 0.1$.

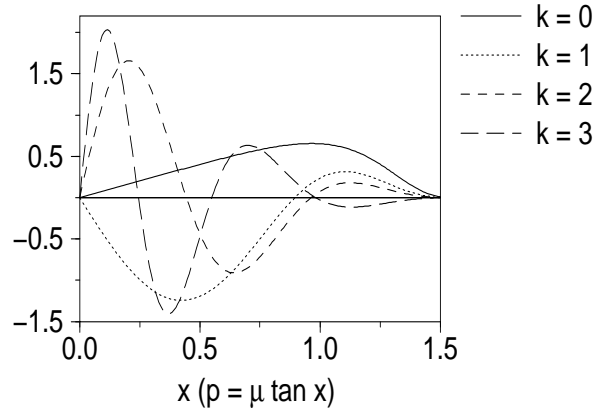


Figure 6: Calculated wave functions in momentum space for the Hulthén potential for the case: $m = 1.0$, $\rho = -0.5$ and $\mu_H = 0.1$.

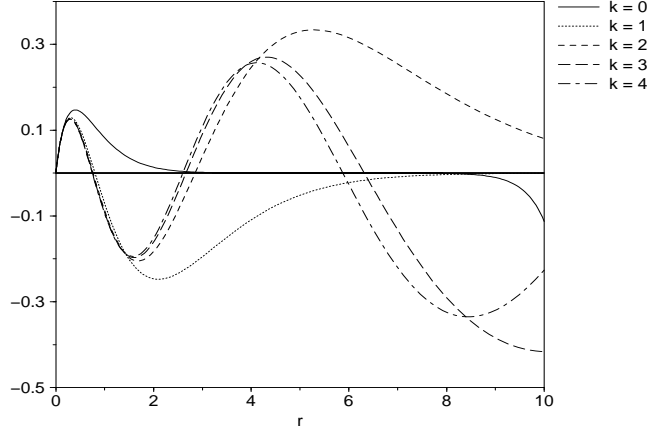


Figure 7: Wave functions calculated for the Hulthén potential by directly solving the differential equation for the case: $m = 1.0$, $\rho = -0.5$ and $\mu_H = 0.1$.

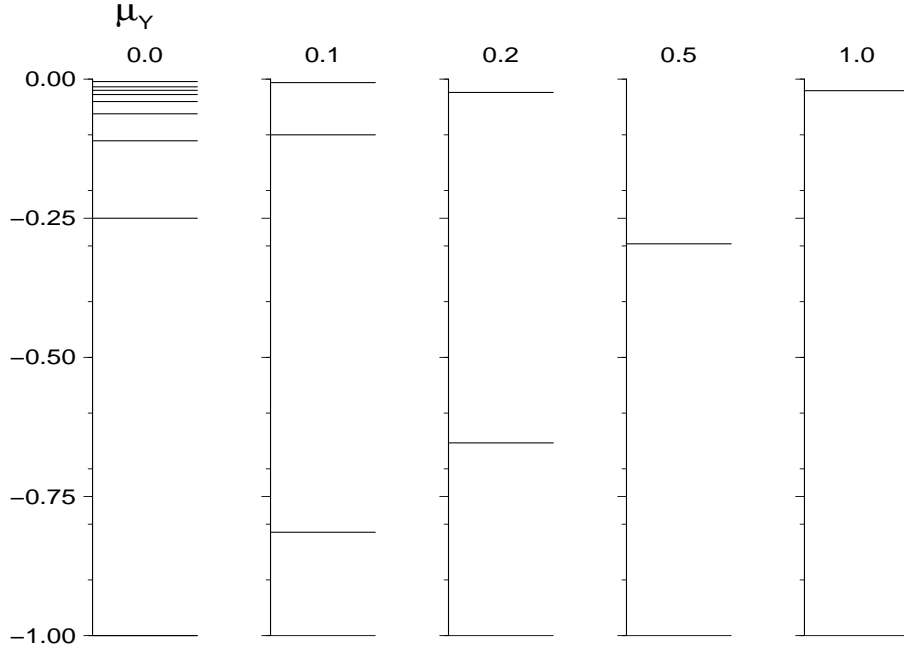


Figure 8: Bound states of a nonrelativistic $q\bar{q}$ system in a Yukawa potential for different values of μ_Y .

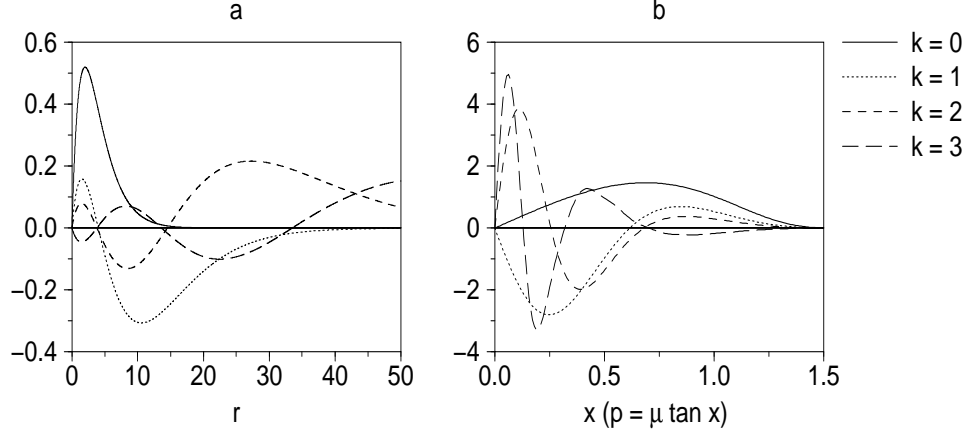


Figure 9: Wave functions in (a) configuration space and (b) momentum space calculated for the Yukawa potential by making an expansion of the eigenfunctions in basis functions for the case: $m = 1.0$, $\rho = -1.0$ and $\mu_Y = 0.02$.

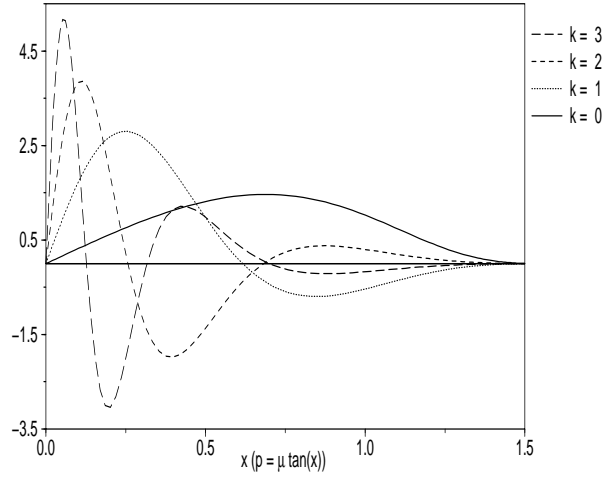


Figure 10: Wave functions in momentum space calculated for the Yukawa potential by directly discretizing the integral equation for the case: $m = 1.0$, $\rho = -1.0$ and $\mu_Y = 0.02$.

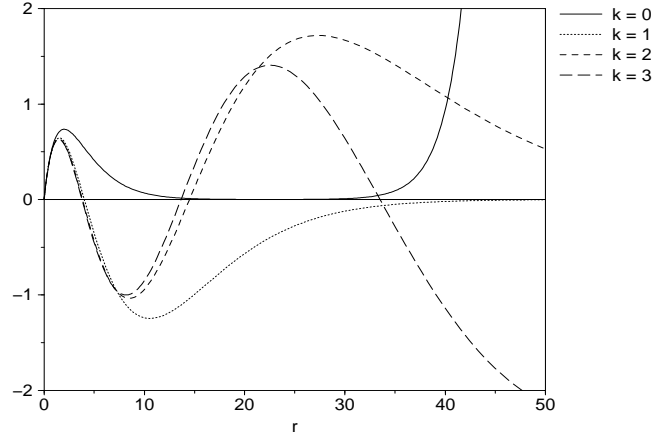


Figure 11: Wave functions in configuration space calculated for the Yukawa potential by directly solving the differential equation for the case: $m = 1.0$, $\rho = -1.0$ and $\mu_Y = 0.02$.

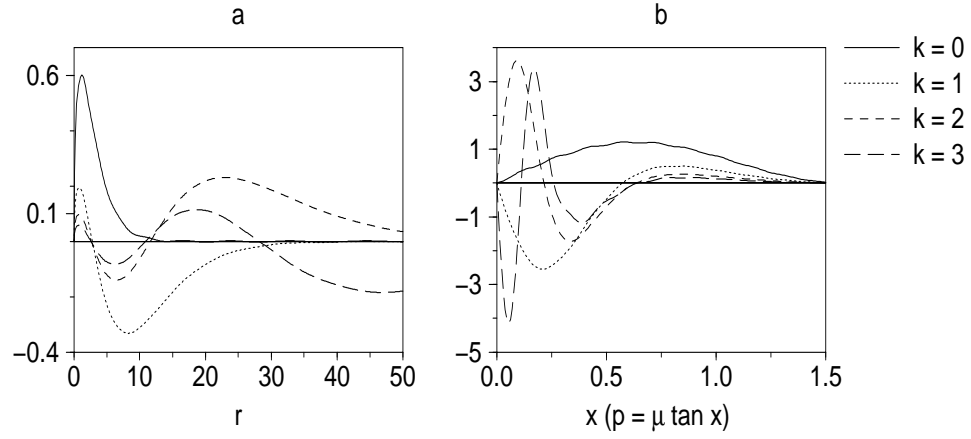


Figure 12: Wave functions for the Yukawa potential by making an expansion in basis functions for the case: $m = 1.0$, $\rho = -1.0$ and $\mu_Y = 0.02$ in the relativistic situation.

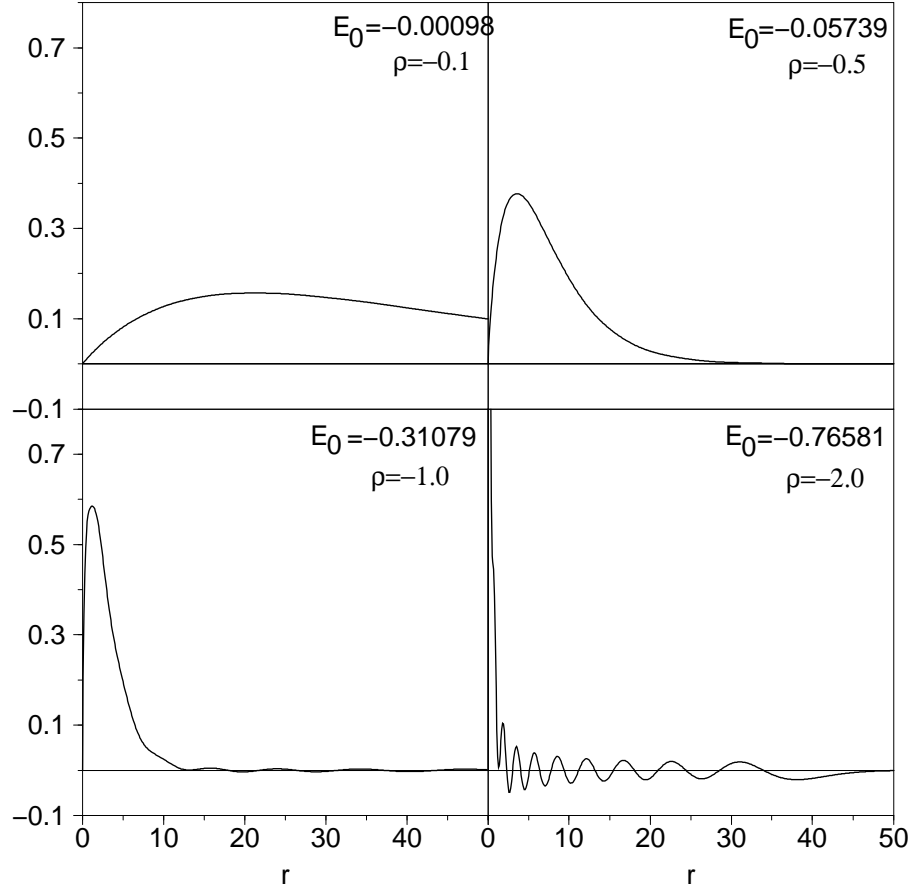


Figure 13: Wave function (relativistic) of the ground state in configuration space for the Yukawa potential with $m = 1.0$, $\mu_Y = 0.02$ and several values of ρ .

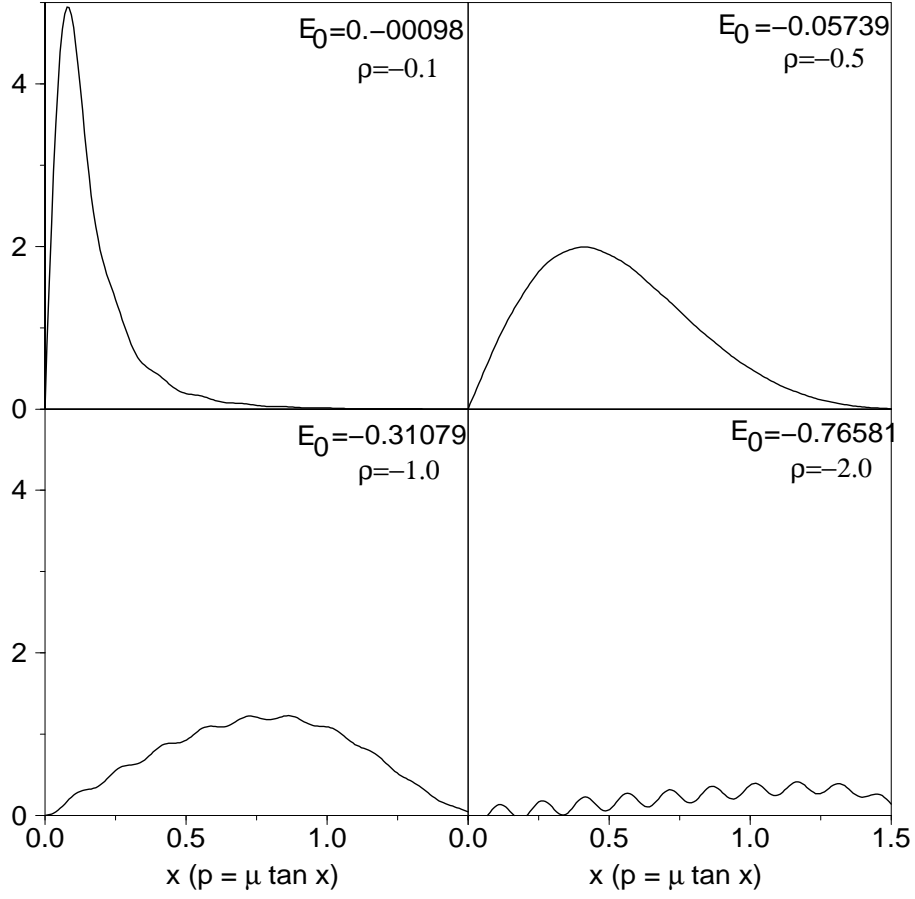


Figure 14: Wave function (relativistic) of the ground state in momentum space for the Yukawa potential with $m = 1.0$, $\mu_Y = 0.02$ and several values of ρ .

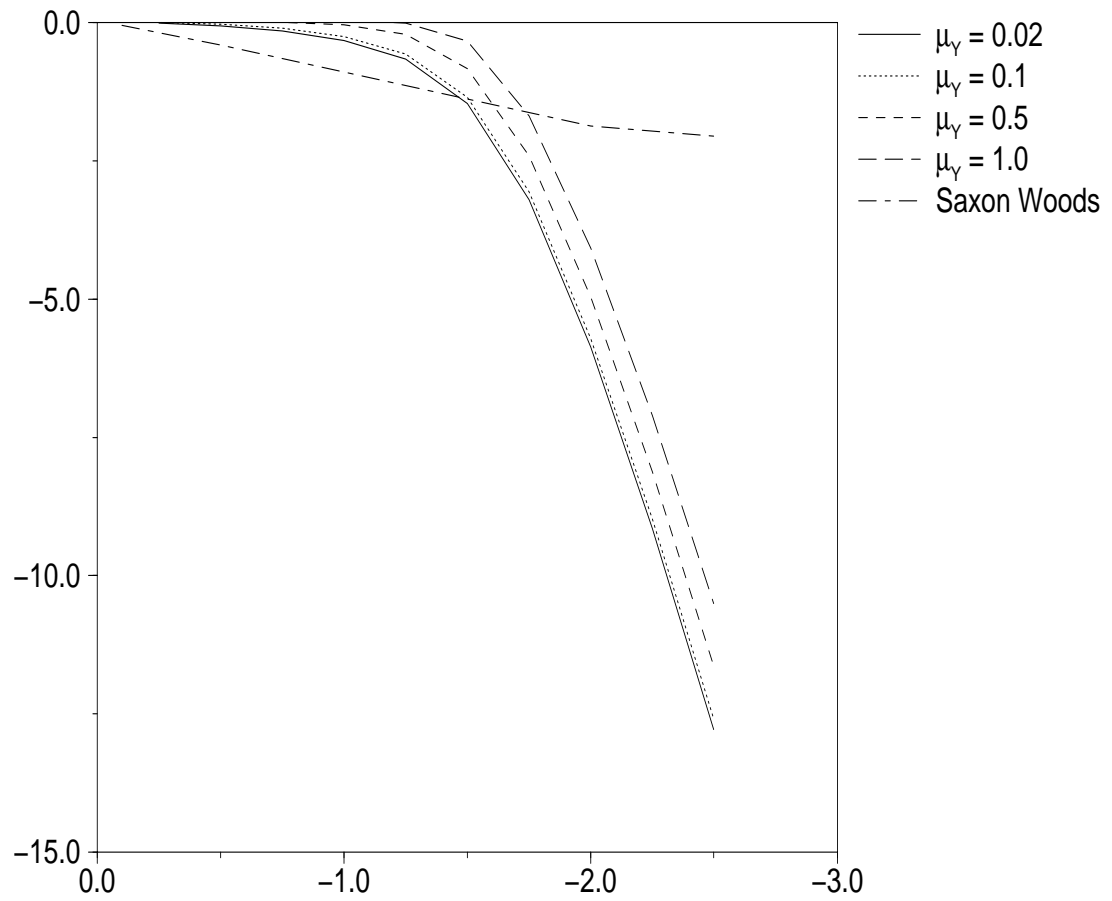


Figure 15: The strength ρ vs. the ground state energy for several values of μ_Y .

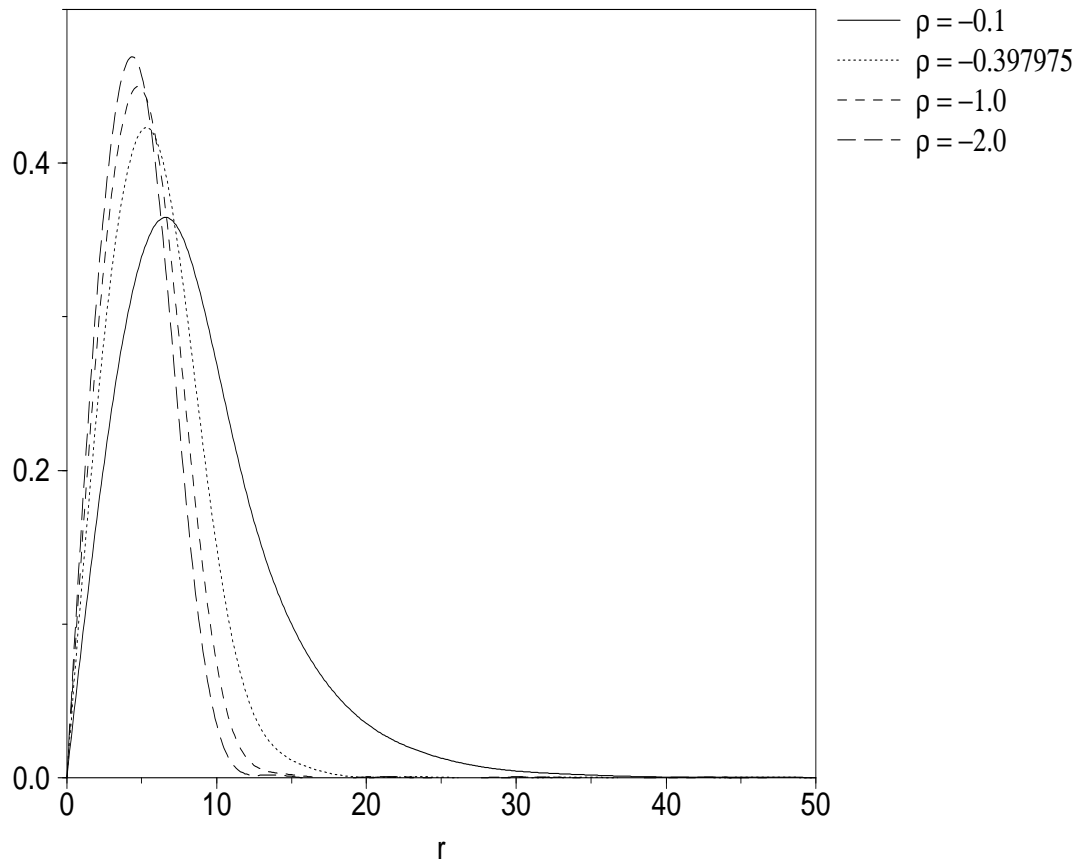


Figure 16: Wave function (relativistic) of the ground state in configuration space for the Saxon Woods potential with $m = 1.0$, $R = 10.0$, $a = 1.0$.

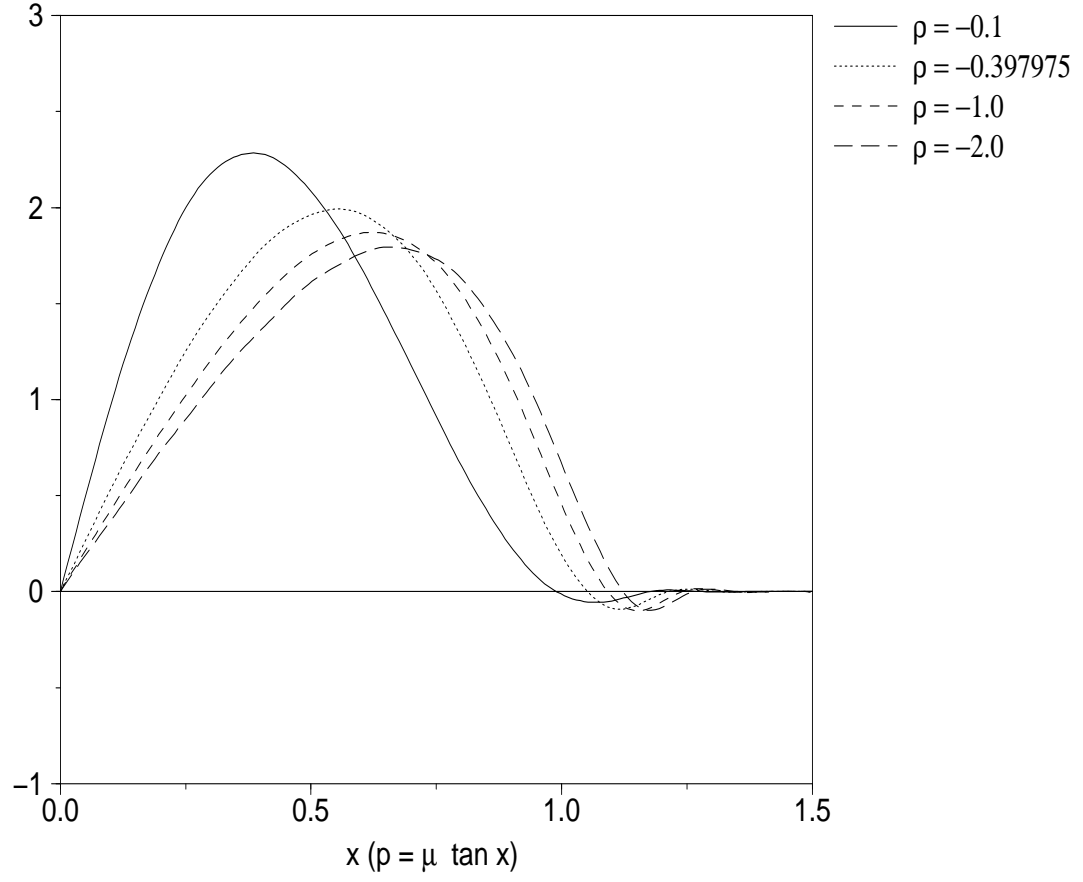


Figure 17: Wave function (relativistic) of the ground state in momentum space for the Saxon Woods potential with $m = 1.0$, $R = 10.0$, $a = 1.0$.